Plasmonically-powered Hot Carrier Induced Light Emission Modulation

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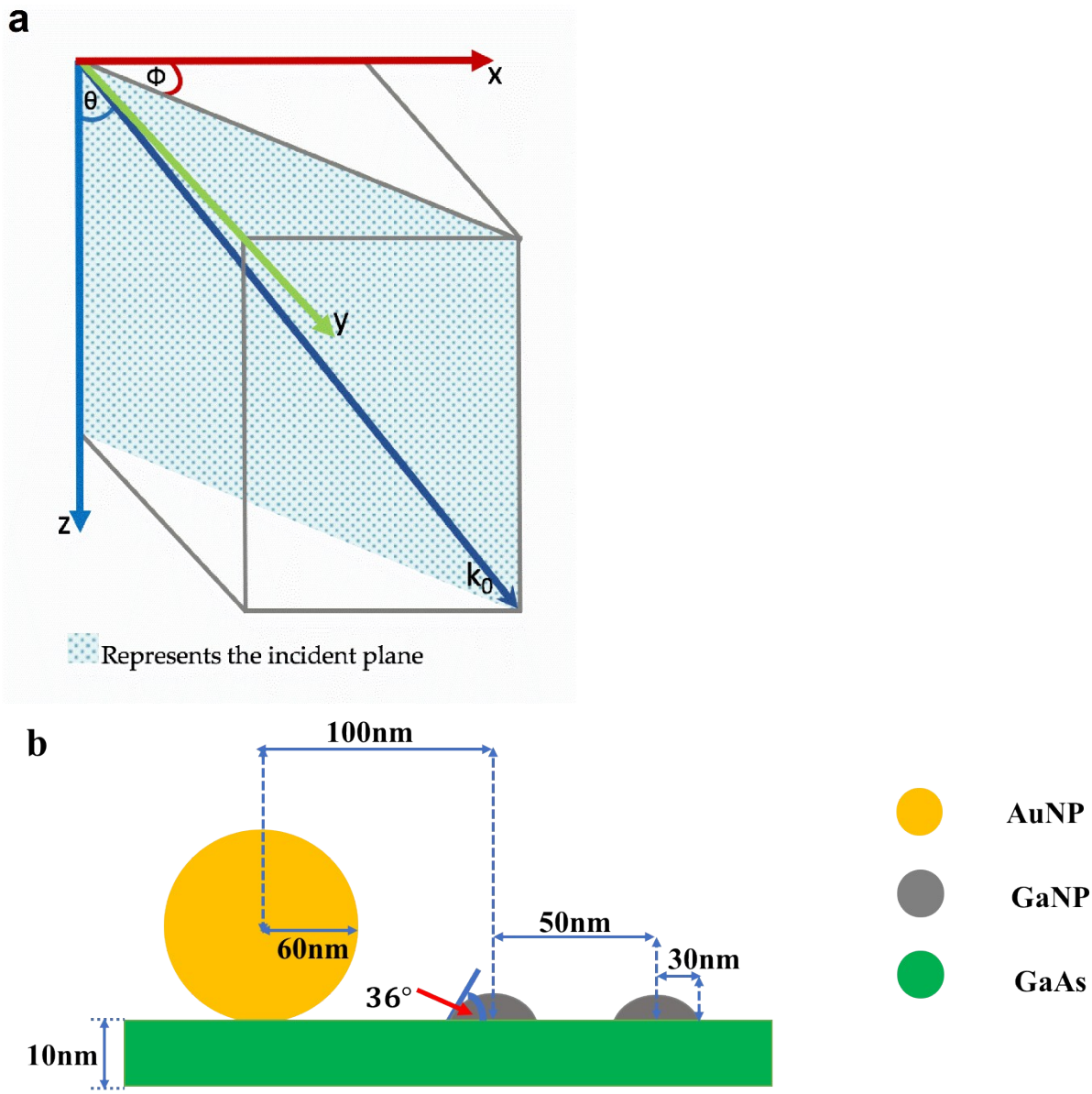
Electromagnetic Modeling

We first model the plasmon field changes between the Ga on GaAs and two species plasmons Ga with Au nanoparticles on GaAs systems is then examined by computational modeling of the former followed by the latter within the visible light range utilizing the RF module of COMSOL Multiphysics®. Theoretically, the 3D models consist of an upper vacuum domain and a lower substrate domain with the nanoparticles (Ga and Au) on the substrate surface. The 60nm diameter Ga nanodroplets subtend a 36° angle with the surface plane of the substrate whiles the Au nanoparticles retain a 120nm diameter. Due to the symmetry of the structures, one cubic cell is studied. A plane wave at 535nm wavelength λ_0, excites the system from the top boundaries off-resonant and the electric field is calculated together with the absorption, reflection and transmission spectra via the finite element method(FEM). The FEM ensures the discretization of the nanoparticle surface instead of the entire volume. For all the systems, the incident and azimuthal angles, θ and φ respectively, relates the Cartesian components of the wavevector by

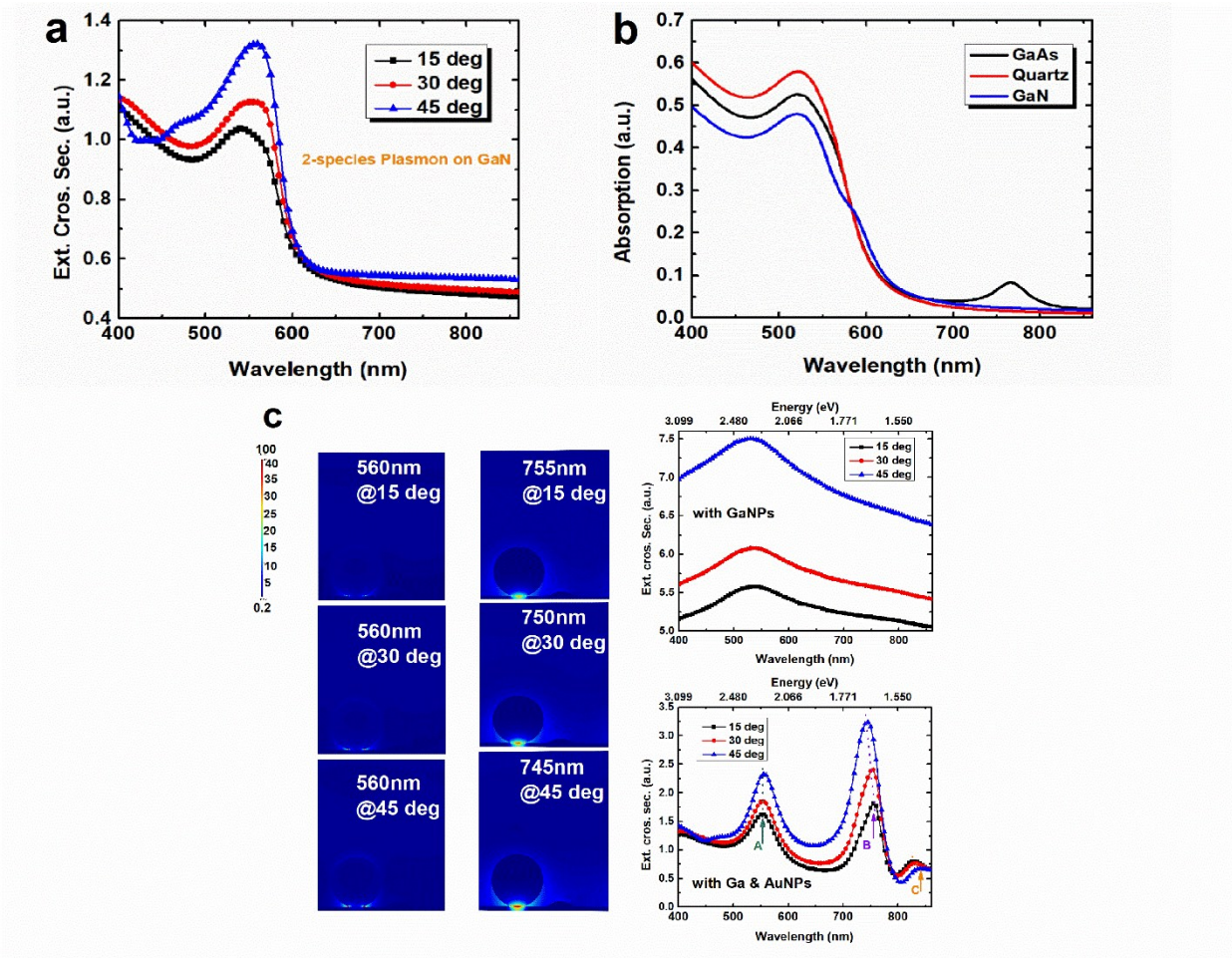
$$k_x = k_0 sin\theta cos\varphi, \; k_y = k_0 sin\theta sin\varphi \text{ and } k_z = k_0 cos\theta \qquad \text{(S1)}$$

θ and φ are set to **0** throughout the calculations which causes the incident plane to be parallel to the xy-plane for normal incidence to the substrate. k_z takes into account the dielectric constant in air, the substrate and at the nanoparticles-substrate interface. The dielectric constant of GaAs is adopted from Aspnes et al.[1] The real and imaginary components of the dielectric function of Ga and Au are interpolated via empirical data from Knight et al.[2] and Johnson and Christy.[3] To replicate semi-infinite layers or periodic structure, the Floquet periodicity boundary

condition(FPBC) is applied to the side surfaces. The FPBC considers the tangential and normal components of the electric fields at the boundaries.



Model schematics. (a) Definition of the incident plane. θ and φ represent the incident and azimuthal direction angles respectively. (b) Dimensions for the electromagnetic modeling (not drawn to scale)



(a) The extinction cross section calculation for the test case of Au+Ga NPs on GaN at varying incidence angle confirming that the higher wavelength peaks are unique to the GaAs substrate. Absorption calculation for varying substrates. (b) Absorption calculation for Au+Ga NPs on GaAs, Quartz and GaN. (c) Calculations for the excitation angle dependent tunability. The third column show the simulated extinction spectra for the single species plasmon system(above) and the two species plasmon system(below). The first and second columns show the calculated field distributions in the two species plasmon system at the extinction peaks A and B respectively for 15°, 30° and 45°incident angles. The peak marked C correspond to the Ga plasmons. The color bar applies to all the field calculations in (c).

References

1. Aspnes, D. E., Kelso, S. M., Logan, R. A. & Bhat, R. Optical properties of AlxGa1−xAs. *J. Appl. Phys.* **60,** 754 (1986).

2. Knight, M. W. *et al.* Gallium plasmonics: Deep subwavelength spectroscopic imaging of single and interacting gallium nanoparticles. *ACS Nano* **9,** 2049–2060 (2015).

3. Johnson, P. B. & Christy, R. W. Optical constants of the noble metals. *Phys. Rev. B* **6,** 4370–4379 (1972).